Screening at Oxide Film and Nanoparticle Surfaces in Electrolyte Solution by MD Simulation

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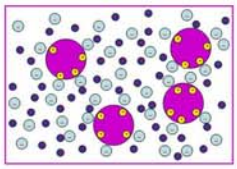
Motivation

Self assembly of nanoparticles in electrolyte solution is controlled by:

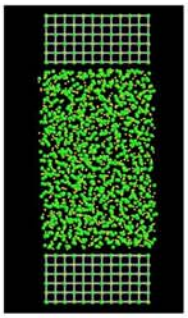
- Surface structure and chemistry
- Nature of solvent: charged, polar or non-polar
- Concentration of nanoparticles and other solute atoms/molecules
- Temperature and pressure of the system



Simulation Model for Ionic Solid-Liquid Interface

- Ionic liquid - NaCl model system interacting via Fumi and Tosi (1964) interionic potential
- Ionic solid - (100) perfect NaCl crystal modeled with Fumi and Tosi potential multiplied by a prefactor, k=50
  - The prefactor raises the melting point by ~k times
- Ionic solid-liquid - interactions are same as ionic liquid
- Ionic liquid is confined between two slabs of ionic solid creating two solid-liquid interfaces
- MD simulations are performed for NVT conditions at 3 different liquid densities

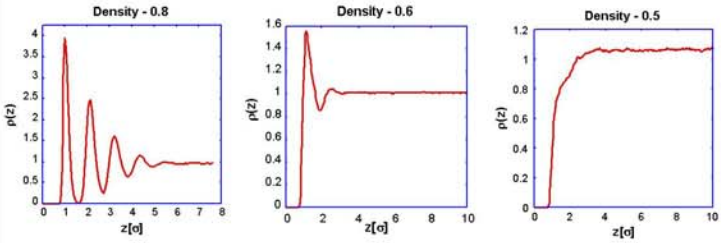
Snapshot of Solid-Liquid Interface



Stable solid-liquid interfaces are seen at T=1600 K and liquid number density of 0.6

Density Distribution across the Interface

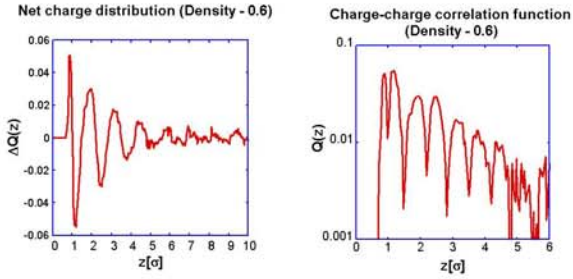
The density distribution function for the liquid is calculated as: $\rho(z)= \rho_+(z) + \rho_-(z)$, where z is the direction normal to interface



It is seen that the *layering* decreases rapidly with decreasing density

Charge Distribution across the Interface

The charge distribution function for the liquid is calculated as: $Q(z)= \rho_+(z) - \rho_-(z)$, where z is the direction normal to interface

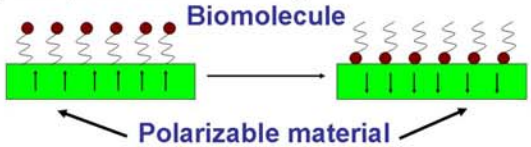


Oscillatory decay of the charge density is a characteristic of screening in dense systems

Future Directions

Computational studies of polarizable barium titanate and lead zirconium titanate surface interaction with biomolecules

- Effect of plane orientation (100),(110) and(111), temperature induced phase transition (tetragonal to cubic phase) and polarization switching



- Comparison with experimental work on biomolecules manipulation on ferroelectric films performed by O. Auciello, M. Firestone (MSD) and L. Ocola (CNM)
- Nanoparticle self-assembly and functionality

1. S. Tinte, M.G. Stachiotti, S. R. Phillpot, M. Sepliarsky, D. Wolf, R. L. Migoni, J.Phys.: Condens.Matter, 16, 3495 (2004)

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